

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) arn039\_150k

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found.      CIF dictionary      Interpreting this report

## Datablock: arn039\_150k

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Bond precision:    C-C = 0.0037 Å

Wavelength=1.34143

Cell:                a=11.4728(3)                b=14.2115(4)                c=16.0992(4)  
                      alpha=92.018(2)        beta=91.054(2)        gamma=112.546(2)  
Temperature:        150 K

	Calculated	Reported
Volume	2421.34(12)	2421.34(12)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	2(C54 H40 Cu N2 O P2), 2(F6 P), C4 H10 O	C54 H40 Cu N2 O P2, F6 P, 0.5(C4 H10 O)
Sum formula	C112 H90 Cu2 F12 N4 O3 P6	C56 H45 Cu F6 N2 O1.50 P3
Mr	2080.80	1040.39
Dx,g cm-3	1.427	1.427
Z	1	2
Mu (mm-1)	3.418	3.409
F000	1070.0	1070.0
F000'	1068.27	
h,k,lmax	14,17,20	14,17,20
Nref	10306	10023
Tmin,Tmax	0.479,0.541	0.406,0.517
Tmin'	0.435	

Correction method= # Reported T Limits: Tmin=0.406 Tmax=0.517

AbsCorr = MULTI-SCAN

Data completeness= 0.973

Theta(max)= 58.164

R(reflections)= 0.0457( 9750)

wR2(reflections)= 0.1269( 10023)

S = 1.032

Npar= 625

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The following ALERTS were generated. Each ALERT has the format

**test-name\_ALERT\_alert-type\_alert-level.**

Click on the hyperlinks for more details of the test.

## ● Alert level C

PLAT220_ALERT_2_C	NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range	3.8 Ratio
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C23 Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C47 Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	51 Report
PLAT918_ALERT_3_C	Reflection(s) with I(obs) much Smaller I(calc) .	9 Check
PLAT927_ALERT_1_C	Reported and Calculated wR2 Differ by .....	-0.0018 Check
PLAT939_ALERT_3_C	Large Value of Not (SHELXL) Weight Optimized S .	14.30 Check

## ● Alert level G

ABSMU01_ALERT_1_G	Calculation of _exptl_absorpt_correction_mu not performed for this radiation type.	
PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	5 Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	5 Report
PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ	Please Check
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.50 Check
PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)	0.002 Degree
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	4 Report
PLAT173_ALERT_4_G	The CIF-Embedded .res File Contains DANG Records	1 Report
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records	3 Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	1 Report
PLAT187_ALERT_4_G	The CIF-Embedded .res File Contains RIGU Records	1 Report
PLAT244_ALERT_4_G	Low 'Solvent' Ueq as Compared to Neighbors of	P3 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O2 Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C55 Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C56 Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C57 Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C58 Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H55A Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H55B Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H56A Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H56B Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H56C Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H57A Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H57B Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H58A Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H58B Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H58C Constrained at	0.5 Check
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 3 )	100% Note
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in ..... (Resd 3 )	7.50 Check
PLAT413_ALERT_2_G	Short Inter XH3 .. XHn H23 ..H58A .	2.00 Ang.
	-1+x,y,z =	1_455 Check
PLAT789_ALERT_4_G	Atoms with Negative _atom_site_disorder_group #	15 Check
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #	2 Note
	F6 P	
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....	13 Note
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .	Please Do !
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	232 Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	6 Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity .....	3.4 Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	9 Info
PLAT984_ALERT_1_G	The C-f' = 0.0148 Deviates from the B&C-Value	0.0137 Check
PLAT984_ALERT_1_G	The Cu-f' = -2.9183 Deviates from the B&C-Value	-2.7974 Check
PLAT984_ALERT_1_G	The F-f' = 0.0600 Deviates from the B&C-Value	0.0583 Check
PLAT984_ALERT_1_G	The N-f' = 0.0253 Deviates from the B&C-Value	0.0241 Check

PLAT984_ALERT_1_G	The O-f' =	0.0412	Deviates from the B&C-Value	0.0389	Check
PLAT984_ALERT_1_G	The P-f' =	0.2596	Deviates from the B&C-Value	0.2543	Check
PLAT985_ALERT_1_G	The Cu-f" =	3.6937	Deviates from the B&C-Value	3.6876	Check
PLAT985_ALERT_1_G	The F-f" =	0.0411	Deviates from the B&C-Value	0.0400	Check
PLAT985_ALERT_1_G	The P-f" =	0.3354	Deviates from the B&C-Value	0.3332	Check

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0 **ALERT level A** = Most likely a serious problem - resolve or explain  
0 **ALERT level B** = A potentially serious problem, consider carefully  
7 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
47 **ALERT level G** = General information/check it is not something unexpected

15 **ALERT type 1** CIF construction/syntax error, inconsistent or missing data  
8 **ALERT type 2** Indicator that the structure model may be wrong or deficient  
5 **ALERT type 3** Indicator that the structure quality may be low  
26 **ALERT type 4** Improvement, methodology, query or suggestion  
0 **ALERT type 5** Informative message, check

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It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special\_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

### Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

### Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

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**PLATON version of 05/12/2020; check.def file version of 05/12/2020**

